

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.40\text{e-}12$ cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: $5.75\text{e-}01$

Confidence level: $5.11\text{e-}01$

Nearest Neighbors from the Training Set

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Methanol

Measured: $9.44\text{e-}13$

Predicted: $1.40\text{e-}12$

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Methylhydrazine

Measured: $6.50\text{e-}11$

Predicted: $2.42\text{e-}11$

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Ethanol

Measured: $3.27\text{e-}12$

Predicted: $4.21\text{e-}12$

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Ethylene oxide

Measured: $7.60\text{e-}14$

Predicted: $2.20\text{e-}13$

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Ethyleneimine

Measured: $6.10\text{e-}12$

Predicted: $9.93\text{e-}12$